Numerical Results for Ground States of Mean-Field Spin Glasses at low Connectivities

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An extensive list of results for the ground state properties of spin glasses on random graphs is presented. These results provide a timely benchmark for currently developing theoretical techniques based on replica symmetry breaking that are being tested on mean-field models at low connectivity. Comparison with existing replica results for such models verifies the strength of those techniques. Yet, we find that spin glasses on fixed-connectivity graphs (Bethe lattices) exhibit a richer phenomenology than has been anticipated by theory. Our data prove to be sufficiently accurate to speculate about some exact results.

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A theoretical understanding of the intricate dynamics of disordered systems has been a major goal of statistical physics at least since the introduction of the Edwards-Anderson spin glass model [1]. Already the study of the equilibrium at low temperature, a state real disordered materials rarely achieve [2], reveals a stunning range of new phenomena, even in the simplest models such as the Sherrington and Kirkpatrick model (SK) where all spins are mutually connected [3, 4, 5, 6]. As an intermediate step in extending the mean-field techniques toward finite-dimensional models, spin glasses on random graphs are an area of active research. Those systems have been of interest from early on because they combine infinite-range connections (like SK) with a finite, decidedly low connectivity. But those earlier studies have focused either on temperatures at the glass transition [7], on purely replica symmetric (RS) solutions [8], or on perturbative approaches in the (SK-)limit of large connectivity [9, 10, 11].

Simultaneously, the formal similarity between spin-glass Hamiltonians and the objective function of combinatorial optimization problems has been realized [12] and exploited to make RS predictions, for instance, for the bipartitioning problem on random graphs [13, 14, 15]. This connection, with the discovery of phase transitions in combinatorial optimization problems [16] and the application of replica techniques to their study [17], has recently rejuvenated interest in spin glasses on random graphs. But to obtain quantitatively valuable predictions for NP-hard problems required the application of replica symmetry breaking (RSB) [5] to those problems at finite connectivities and low temperatures which was accomplished recently [18, 19, 20]. Finally, these RSB methods are now being applied to spin glasses on random graphs, producing quantitatively valuable results [18, 21] at accuracies below 0.1%. At this level of accuracy, a comparison between theoretical and simulation results becomes valuable at least in two respects: Convergence of the numerical with the RSB result can verify the assumptions underlying RSB as well as the quality of the numerical method used to approximate an NP-hard problem.

In this letter we apply the extremal optimization (EO) heuristic [22, 23] to investigate the ground state properties of spin glasses on random graphs. With this method we have sampled system sizes up to $n = 4096$ on low-connectivity graphs. We have obtained high-accuracy results for the ground-state energies of spin glasses on ordinary random graphs (ORG) with fluctuating connectivities, and for Bethe-lattice graphs (BL) with fixed connectivities. On a smaller sample of BL, we have also obtained results for the entropy of such graphs. The energies are in excellent agreement with RSB predictions for low-connectivity BL [21]. Both, the energies and entropies reveal a sensitivity to the even-oddness of the BL, which may explain inconsistencies with results in the SK limit [9]. No such inconsistency arises for ORG and the numerical extrapolation is in good agreement with analytic results for the large-connectivity limit in RSB [9]. The BL energies seem to fall (within 0.2%) on a simple line ranging from the 2-connected graphs to the SK-limit, but only for *even integer* connectivities, without any obvious interpolation. The BL entropies decrease linearly with the inverse connectivity for odd connectivities, but are already consistent with zero (within accuracy) at small even connectivity. More details of the numerical procedure is given elsewhere [24, 25].

Of the two types of random graphs are considered for this study, the BL are regular random graphs [26]. These graphs consist of n vertices where each vertex possesses a fixed number $k+1$ of bonds [13, 18, 21] with randomly selected other vertices. Alternatively, ORG are obtained by randomly connecting any pair of vertices with a specified probability $p = c/(n-1)$, leading to a graph of average connectivity c but where the connectivities of individual vertices are Poissonian distributed [26]. Note that each vertex' connectivity, and thus $k+1$, is inherently discrete, while c can take on any real value.

Once a graph of connectivity c is generated, randomly chosen quenched couplings $J_{i,j} \in \{-1, +1\}$ are assigned to existing bonds between neighboring vertices i and j. Each vertex i is occupied by a spin variable $x_i \in \{-1, +1\}$. The energy of the system is defined as

the difference in number between violated bonds and satisfied bonds, $H = -\sum_{\{bonds\}} J_{i,j} x_i x_j$, and we will focus on the energy and entropy per spin, resp.,

$$e_c = \frac{1}{n} H, \qquad s_c = \frac{1}{n} \ln \Omega, \qquad (1)$$

where Ω is the degeneracy of the configurations exhibiting the ground state energy.

For our numerical procedure we used the following implementation of EO [22, 23]: For a given spin configuration on a graph, assign to each spin x_i a "fitness" $\lambda_i = -\#violated\ bonds = -0, -1, -2, \ldots, -c_i$, so that $e_c = -\sum_i \lambda_i/(2n)$ is satisfied. Here, c_i is the integer connectivity of vertex i, and $c_i \equiv k + 1$ for every vertex in BL. If $c_{\max} = \max_i c_i$, each spin falls into one of only $c_{\max} + 1$ possible states. Say, currently there are $n_{c_{\max}}$ spins with the worst fitness, $\lambda = -c_{\max}$, $n_{c_{\max}-1}$ with $\lambda = -c_{\max} + 1$, and so on up to n_0 spins with the best fitness $\lambda = 0$, where $\sum_j n_j = n$. Now draw a "rank" l according to the distribution $P(l) \sim l^{-\tau}$. Then, determine $0 \leq j \leq c_{\max}$ such that $\sum_{i=j+1}^{c_{\max}} n_i < l \leq \sum_{i=j}^{c_{\max}} n_i$. Finally, select any one of the n_j spins in state j and reverse its orientation *unconditionally*. As a result, it and its neighboring spins change their fitness. After all the effected λ's and n's are reevaluated, a new spin is chosen for an update.

The arguments given in [27] and a few experiments indicate that $\tau = 1.3$ is a satisfactory choice to find ground states efficiently on either type of graph. Our implementation restarts for each instance at least $r_{\max} = 4$ times with new random initial spin assignments, executing $\approx 0.1\, n^3$ updates per run. If a new, lower-than-previous energy state is encountered in run r, we adjust $r_{\max} = 2 + 2r$ for that instance so that EO runs at least twice as many restarts as were necessary to find the lowest state in the first place. Especially for small n, $r_{\max}$ hardly ever exceeds 4; for larger n a few graphs require up to 30 restarts before termination. Since EO perpetually explores new configurations it is well suited to explore also the degeneracy Ω of low-energy states. In these runs, we used a similar approach to the above, except for setting $r_{\max} = 8 + 2r$, where r is the latest run in which a new configuration of the lowest energy was located.

We have simulated spin glasses on BL with this algorithm for $k + 1$ between 3 and 26, and graph sizes $n = 2^l$ for $l = 5, 6, \ldots, 10$ to obtain results for ground state energies [24]. In particular, for $k + 1 = 3$ we have used the methods described in Ref. [25] to reach system sizes of $n = 4096$. In a separate simulation, using $\tau = 1.4$, we have explored BL of size $n \in [16 \ldots 256]$ to determine their entropy. We have used the same algorithm, preceded by a graph reduction procedure [25], to study ORG ranging from $n \leq 2^{15}$ for $c = 2$ to $n \leq 2^9$ at $c = 25$. Amazingly, as is shown in Refs. [24, 25], in all these cases
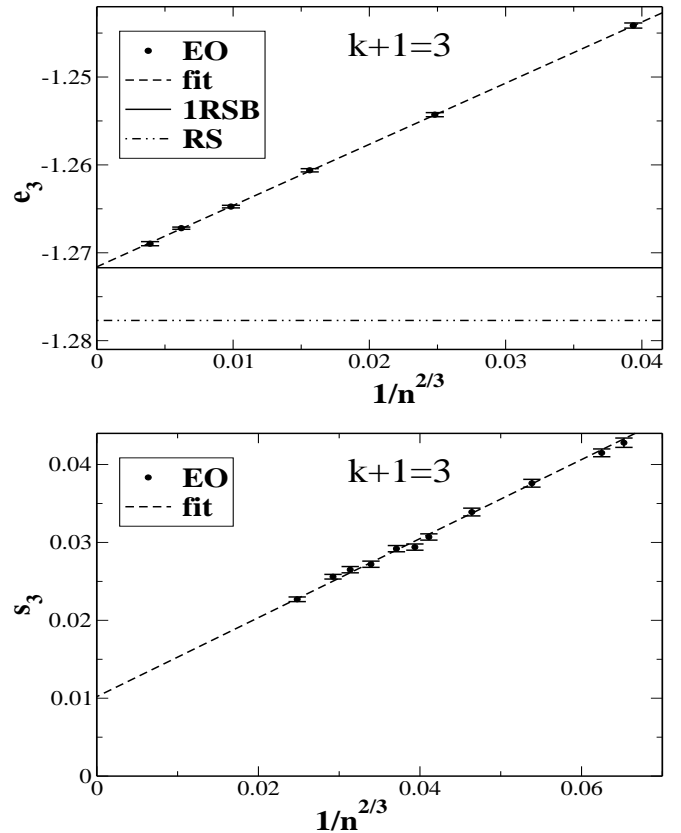

FIG. 1: Extrapolation plot for the BL energies (above) and entropies (below) for $k + 1 = 3$ obtained with EO for finite n [24]. The data is plotted vs. $1/n^{2/3}$ and is fitted according to Eq. (2). (Data points were weighted with respect to n and the inverse of the error.) For $n \to \infty$ the extrapolation for the energy gives $e_3 = -1.2716(1)$, way above the RS result but consistent with the 1RSB result [21], both indicated by horizontal lines. The extrapolation for the entropy gives $s_3 = 0.0102(10)$.

our data can be extrapolated for $n \to \infty$ via

$$e_c(n) \sim e_c + \frac{A}{n^{2/3}} \quad (n \to \infty). \qquad (2)$$

Deviations from these scaling corrections are generally small [24] and we assume Eq. (2) to be exact here. There does not appear to be a theoretical justification for Eq. (2), but in Fig. 1 we show representatively the large-n extrapolation of our data for $k + 1 = 3$. Both, finite-n energies and entropies, appear to scale linearly when plotted for $1/n^{2/3}$. The extrapolation results for the energies of BL and ORG are given in Tab. I. The extrapolation results for the BL entropies are given in Tab. II. Variation in the (estimated) errors reflect differences in computational effort (number of instances, largest n) and in the quality of the extrapolation [24].

We can compare our results with existing theoretical predictions at the RS and the 1RSB level at least for the case of BL at $k + 1 = 3$. For this case, Ref. [21] reproduced $e_3 = -1.2777$ at the RS level, and yielded

TABLE I: Extrapolated energies per spin for BL (left) and ORG (right). Although only integer values of the average connectivity c were considered, it can take on any real value, unlike $k + 1$.

$k+1$	e_{k+1}	$k+1$	e_{k+1}	c	e_c
3	-1.2716(1)	12	-2.6127(9)	2	-0.9192(2)
4	-1.472(1)	14	-2.8287(5)	3	-1.2059(2)
5	-1.673(1)	15	-2.935(1)	4	-1.4311(10)
6	-1.826(1)	16	-3.0268(9)	5	-1.6224(10)
7	-1.991(3)	18	-3.212(2)	10	-2.356(3)
8	-2.1213(9)	20	-3.389(1)	15	-2.906(5)
9	-2.2645(5)	25	-3.806(4)	20	-3.373(5)
10	-2.378(3)			25	-3.775(8)

TABLE II: Extrapolated entropies per spin for BL.

$k+1$	s_{k+1}	$k+1$	s_{k+1}
3	0.0102(10)	4	0.0381(15)
5	0.0048(10)	6	0.0291(10)
7	0.0020(10)	8	0.0218(10)
9	0.0002(15)	10	0.0198(10)
14	0.0126(10)	15	0.0002(15)
18	0.0095(10)	22	0.0076(10)
26	0.0063(15)		

$e_3 = -1.2717$ at the 1RSB level (further replica corrections are expected to be small). These values and our extrapolation result of $e_3 = -1.2716(1)$ are indicated in Fig. 1. Clearly, the extrapolation result is extremely close to the 1RSB results, but inconsistent with the RS result.

We have also used EO to sample the degeneracy Ω of the lowest-energy states found for BL. In these simulations we focused on smaller system sizes of $n \leq 256$ for $k+1 = 3, \ldots, 9$ and $10, 14, \ldots, 26$ only. As a test for the accuracy of our implementation, we have run the simulation for $k + 1 = 3$ a second time on identical instances, using different initial conditions and $n/5$ more updates, obtaining identical results *for each instance*.

When plotted for $1/(k + 1)$ in Fig. 2, the BL entropies for even connectivities decrease about linearly toward zero. The entropies for odd connectivities, clearly non-zero at $k + 1 = 3$ (see Fig. 1), drop more rapidly and are essentially indistinguishable from zero already at $k + 1 = 9$. While any rapid, smooth decay could easily escape our limited accuracy, the plot still raises the question whether there may be a finite connectivity beyond which odd entropies vanish. The qualitative difference between even and odd BL entropies can be understood in the presents or absence, resp., of "free spins," a finite fraction of spins in the ground state which violate exactly half of their bonds and may flip at no cost [24].

We have also plotted all BL and ORG energies as $e_c/\sqrt{c}$ vs. $1/c$ (where $c = k + 1$ for BL) in Fig. 3. We
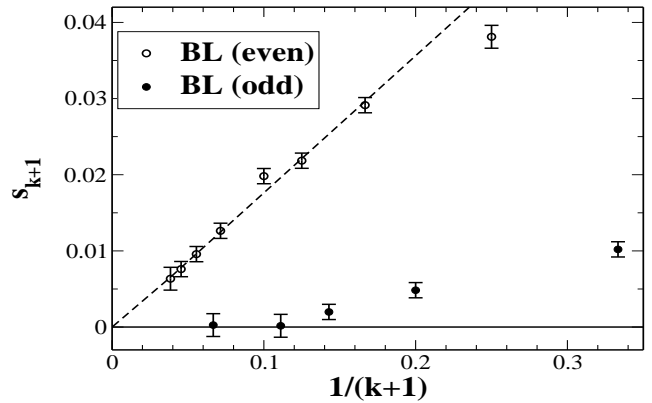

FIG. 2: Asymptotic plot of the extrapolated entropies from Tab. II as a function of $1/(k+1)$. The data for even $k+1$ seems to vanish linearly with $1/(k + 1)$ (dashed line). The data for odd $k + 1$ drops more precipitously, and can not reasonably be fitted at this level of accuracy.

expect that $\lim_{c \to \infty} e_c/\sqrt{c} = E_{SK} = -0.76321$ for RSB [6, 28]. All energies for ORG appear to fall on a single smooth curve. We can fit those energies with a parabola, projecting $E_{SK}^{ORG} \approx -0.761$. In contrast, the BL energies split into even and odd values, each located apparently on a simple line. Each line separately extrapolates very close to the exact value: $E_{SK}^{even} \approx -0.763$ and $E_{SK}^{odd} \approx -0.765$. Amazingly, the trivial value of $e_2 = -1$ is very close to the linear fit for the even results. Clearly, a function that would interpolate continuously *all* the BL energies will have to be very complicated (oscillatory). But we may speculate that its envelope for the even e_{k+1} is a simple line, passing $e_2 = -1$ and the SK result:

$$\mathcal{E}_{k+1} = E_{SK}\sqrt{k + 1} - \frac{2E_{SK} + \sqrt{2}}{\sqrt{k + 1}}. \qquad (3)$$

In Fig. 4 we plot the deviation $\epsilon = e_{k+1}/\mathcal{E}_{k+1} - 1$ of the extrapolated energies from Eq. (3) for even $k + 1$. While the extrapolated values do not fall exactly onto the proposed function, they are *all* within about 0.2% of it. In fact, all points are slightly too high, which may indicate a more complex functional correction to Eq. (3), or a systematic error, say, in the extrapolation due to higher-order corrections.

It has been pointed out [29] that Eq. (3) would imply that a first-order perturbation around the trivial $k+1 = 2$ solution would be exact and give the RSB result for the SK model. But the obvious continuation of BL off the even integers fails to interpolate the data smoothly. If we "interpolate" BL for each $k + 1 = 2, 4, 6, \ldots$ with a mix of $(1-p)n$ $(k+1)$-vertices and pn $(k+3)$-vertices for $0 \leq p \leq 1$, the resulting energies only provide a set of *secants*, $e_{k+1+2p} = pe_{k+3} + (1-p)e_{k+1}$, to the even-integer data. We have also plotted our (somewhat less accurate) extrapolation results for those interpolating graphs in Fig. 4. On this scale, the singular behavior of this
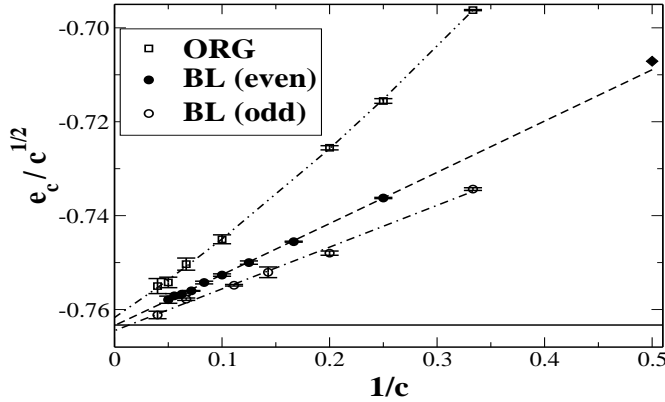
It will be most interesting to see how well upcoming RSB calculations at $T = 0$ for even $k + 1$ will correspond to the proposed function in Eq. (3), or to the extrapolated energies in Tabs. I in general. While the EO algorithm in itself can not provide information about the physics at $T > 0$, the results presented in this Letter are sufficiently promising to apply EO also to sample other models [23] and more complicated properties of the ground states, such as overlap distributions and excitations.

FIG. 3: Plot of the rescaled extrapolated energies, $e_c/\sqrt{c}$, as a function of $1/c$ for ORG (squares) and BL (circles), where $c = k + 1$. The BL data appears to fall on two separate straight lines for even and for odd $k + 1$, *including* the trivial result, $e_2 = -1$ (diamond). In all cases, the fits (dashed lines) provide an reasonable estimate for $E_{SK} = -0.76321$ (horizontal line) at infinite connectivity.
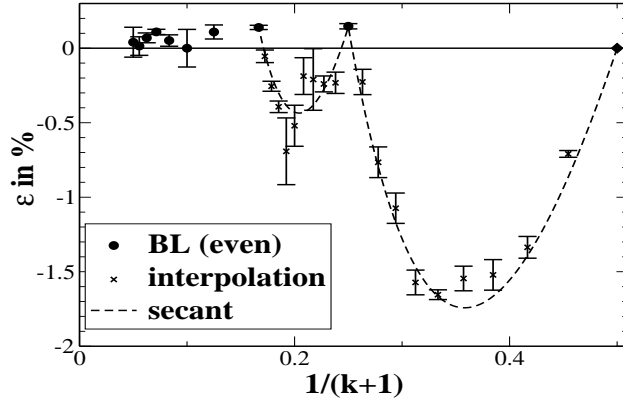

FIG. 4: Plot of the deviation ϵ of the BL energies for even $k + 1$ (circles) relative to Eq. (3) as a function of $1/(k + 1)$. All BL data deviates *at worst by 0.2%*. The point at $k + 1 = 2$ (diamond) is exact. Energies from the interpolating graphs (crosses) do not smoothly interpolate the BL data. Dashed lines are derived from the secants $e_{k+1+2p} = p e_{k+3} + (1 - p)e_{k+1}$, $k + 1 = 2, 4$ and $0 \le p \le 1$, and clearly trace the interpolating data.

continuation at the even integers becomes obvious.

We can further compare our extrapolated energies with perturbative calculations in the SK-limit of infinite connectivity [9, 10, 11]. A recent RSB calculation indicates a $1/c$-correction for the ground state energy of $f_1^{BL} \approx -0.32$ for BL and $f_1^{ORG} \approx 0.17$ for ORG (see Figs. 3 and 4 of Ref. [9]). While our (crude) fit in Fig. 3 predicts a slope at the origin of ≈ 0.16 for ORG, the slopes for either even or odd BL data would predict $\approx 0.11 - 0.10$, or 0.1122 from Eq. (3), far from the perturbative result. It appears that the oscillation between even and odd $k + 1$ complicates also the analytic continuation of the BL problem for large connectivities.

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